L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR

G1 H, Me, n-Pr, n-Bu

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 17:17:25 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS 2 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 2 TO 124 PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

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L2 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2010 ACS on STN

RN 869114-04-5 REGISTRY

ED Entered STN: 01 Dec 2005

CN D-arabino-Hexitol, 1,5-anhydro-2,4,6-trideoxy-2-[[(4-methoxyphenyl)methyl]amino]-6,6-diphenyl-, ethanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H29 N O3 . C2 H2 O4

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 862647-22-1

CMF C26 H29 N O3

Absolute stereochemistry. Rotation (-).

CM 2

CRN 144-62-7 CMF C2 H2 O4

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2010 ACS on STN

RN 805251-49-4 REGISTRY

ED Entered STN: 30 Dec 2004

CN 2H-Pyran-3-amine, 6-(diphenylmethyl)tetrahydro-N-(phenylmethyl)-, (3R,6R)-rel- (CA INDEX NAME)

FS STEREOSEARCH

MF C25 H27 N O

CI COM

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 4.69 4.91

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 17:17:36 ON 23 FEB 2010 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 23 Feb 2010 VOL 152 ISS 9
FILE LAST UPDATED: 22 Feb 2010 (20100222/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Dec 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Dec 2009

CAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 12 L3 4 L2

=> d 1-4 bib abs hitstr

- L3 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN
- AN 2008:825727 CAPLUS
- DN 149:152940
- TI Preparation of trisubstituted benzhydryl-benzylamino-pyranols and 3,6-disubstituted pyran derivatives as monoamine reuptake inhibitors for treating depression
- IN Dutta, Aloke K.
- PA Wayne State University, USA
- SO U.S. Pat. Appl. Publ., 54pp., Cont.-in-part of U.S. Ser. No. 330,972. CODEN: USXXCO
- DT Patent
- LA English
- FAN. CNT 6

FAIN.	PATENT NO.				KIND		DATE			APPLICATION NO.					DATE			
PI	US 2	0030	0225			A1 A1		2008 2003	1204		US 2 US 2			_			00800	
	US 6995268 WO 2005105075			B2 2006020 ⁻ A1 20051110				WO 2005-US12748						20050415				
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
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EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG US 20060122263 US 2006-330972 20060608 20060112 Α1 PRAI US 2003-311796 20030328 A2 US 2004-563189P Р 20040416 WO 2005-US12748 A2 20050415 US 2006-330972 A2 20060112 US 2000-212921P Ρ 20000620 WO 2001-US40964 W 20010614 ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT MARPAT 149:152940 GΙ

Novel 3,6-disubstituted pyrans (I, A, A', and B = optionally substituted AB C4-C14 aryl and heteroaryl wherein heteroatoms of heteroaryl A and/or A' are selected from the group consisting of O, N, and S; Z = a chemical bond and Y-(CH2)o wherein Y = NH or O and o = 0-4; R = H or C1-8 alkyl; W = H or OH; and n and m = 0-4, and wherein any carbon of -(CH2)n may be substituted by OR4 wherein R4 = C1-8 alkyl, C2-18 alkylene, or COOR5 wherein R5 = $\overline{\text{C1-8}}$ alkyl or C2-18 alkylene) or a pharmaceutically acceptable derivative or salt, are monoamine reuptake inhibitors with activity profiles of antidepressants. The synthesis of the pyrans is exemplified. For example, cis(6-benzhydryltetrahydropyran-3-yl)(2-indolemethyl)amine (II) was prepared by reacting trans-5-amino-2-diphenylmethyltetrahydropyran with 2-indolecarboxaldehyde followed by reduction with NaCNBH3. The affinity of II in binding to rat dopamine transporter, serotonin transporter, and norepinephrine transporter was assessed by measuring inhibition of binding of (3H)WIN 35,428, (3H)citalopram, and (3H)nisoxetine, resp.; II had IC50's of 227, 1640, and 401 nM, resp.

IT 805251-49-4P 869114-04-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of trisubstituted benzhydryl-benzylamino-pyranols and 3,6-disubstituted pyran derivs. as monoamine reuptake inhibitors for treating depression)

RN 805251-49-4 CAPLUS

CN 2H-Pyran-3-amine, 6-(diphenylmethyl)tetrahydro-N-(phenylmethyl)-, (3R,6R)-rel- (CA INDEX NAME)

Relative stereochemistry.

RN 869114-04-5 CAPLUS

CN D-arabino-Hexitol, 1,5-anhydro-2,4,6-trideoxy-2-[[(4-methoxyphenyl)methyl]amino]-6,6-diphenyl-, ethanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 862647-22-1 CMF C26 H29 N O3

Absolute stereochemistry. Rotation (-).

CM 2

CRN 144-62-7 CMF C2 H2 O4

L3 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN

AN 2006:544664 CAPLUS

DN 145:27854

TI Preparation of trisubstituted benzhydryl-benzylamino-pyranols and 3,6-disubstituted pyran derivatives as monoamine reuptake inhibitors for treating depression

IN Dutta, Aloke K.

PA USA

SO U.S. Pat. Appl. Publ., 57 pp., Cont.-in-part of U.S. Ser. No. 311,796. CODEN: USXXCO

DT Patent

LA English

FAN.CNT 6

	PATENT NO.				KIN	D	DATE			APPLICATION NO.						DATE			
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PRAI US 2003-311796
                                   20030328
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     US 2004-563189P
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     WO 2005-US12748
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                                   20050415
     US 2000-212921P
                            Ρ
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     WO 2001-US40964
                                   20010614
                            W
     US 2006-330972
                            Α
                                   20060112
     WO 2007-US60455
                                   20070112
                            W
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
     MARPAT 145:27854
OS
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GΙ

Novel 3,6-disubstituted pyrans (I, wherein A and A' = optionally substituted C4-C14 aryl and heteroaryl; Z = a chemical bond and Y-(CH2)o wherein Y = NH or O and o = 0-4; R = H, C1-8 alkyl, C2-8 alkenyl, or C2-8 alkynyl; W = H or OH; B= (un)substituted C4-C14 aryl and C4-C14 heteroaryl; and n and m = 0-4, and wherein any carbon of -(CH2)n may be substituted by OR4 wherein R4 = C1-8 alkyl, C2-18 alkylene, or COOR5 wherein R5 = C1-8 alkyl or C2-18 alkylene) or a pharmaceutically acceptable derivative or salt, are monoamine reuptake inhibitors with activity profiles of antidepressants. The synthesis of the pyrans is exemplified. For example, cis(6-benzhydryltetrahydropyran-3-yl)(2-indolemethyl)amine (II) was prepared by reacting trans-5-amino-2-diphenylmethyltetrahydropyran with 2-indolecarboxaldehyde followed by reduction with NaCNBH3. The affinity of II in binding to rat dopamine transporter, serotonin transporter, and norepinephrine transporter was assessed by measuring inhibition of binding

of (3H)WIN 35,428, (3H)citalopram, and (3H)nisoxetine, resp.; II had IC50's of 227, 1640, and 401 nM, resp.

ΤТ 805251-49-4P 869114-04-5P

> RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(drug candidate; preparation of trisubstituted benzhydryl-benzylamino-pyranols and 3,6-disubstituted pyran derivs. as monoamine reuptake inhibitors for treating depression)

RN 805251-49-4 CAPLUS

2H-Pyran-3-amine, 6-(diphenylmethyl)tetrahydro-N-(phenylmethyl)-, CN (3R,6R)-rel- (CA INDEX NAME)

Relative stereochemistry.

RN 869114-04-5 CAPLUS

CN D-arabino-Hexitol, 1,5-anhydro-2,4,6-trideoxy-2-[[(4methoxyphenyl)methyl]amino]-6,6-diphenyl-, ethanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 862647-22-1 CMF C26 H29 N O3

Absolute stereochemistry. Rotation (-).

CM 2

CRN 144-62-7 CMF C2 H2 O4

ANSWER 3 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN L3

2005:1195739 CAPLUS ΑN

DM 143:460030 TI Preparation of trisubstituted benzhydryl-benzylamino-pyranols and 3,6-disubstituted pyran derivatives as monoamine reuptake inhibitors for treating depression

IN Dutta, Aloke K.

PA Wayne State University, USA

SO PCT Int. Appl., 112 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 6						ETNI	n	רא יי ב			APPLICATION NO.						רע בר		
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ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT OS CASREACT 143:460030; MARPAT 143:460030

$$(CH_2)_n - NR$$
 $(CH_2)_m$
 B
 A

AB Novel 3,6-disubstituted pyrans (I, A, A', and B = optionally substituted C4-C14 aryl and heteroaryl wherein heteroatoms of heteroaryl A and/or A' are selected from the group consisting of O, N, and S; Z = a chemical bond and Y-(CH2)o wherein Y = NH or O and o = 0-4; R = H or C1-8 alkyl; W = H or OH; and n and M = 0-4, and wherein any carbon of -(CH2)n may be substituted by OR4 wherein R4 = C1-8 alkyl, C2-18 alkylene, or COOR5 wherein R5 = C1-8 alkyl or C2-18 alkylene) or a pharmaceutically

acceptable derivative or salt, are monoamine reuptake inhibitors with activity profiles of antidepressants. The synthesis of the pyrans is exemplified. For example, cis(6-benzhydryltetrahydropyran-3-yl)(2-indolemethyl)amine (II) was prepared by reacting trans-5-amino-2-diphenylmethyltetrahydropyran with 2-indolecarboxaldehyde followed by reduction with NaCNBH3. The affinity of II in binding to rat dopamine transporter, serotonin transporter, and norepinephrine transporter was assessed by measuring inhibition of binding of (3H)WIN 35,428, (3H)citalopram, and (3H)nisoxetine, resp.; II had IC50's of 227, 1640, and 401 nM, resp.

IT 805251-49-4P 869114-04-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of trisubstituted benzhydryl-benzylamino-pyranols and 3,6-disubstituted pyran derivs. as monoamine reuptake inhibitors for treating depression)

RN 805251-49-4 CAPLUS

CN 2H-Pyran-3-amine, 6-(diphenylmethyl)tetrahydro-N-(phenylmethyl)-, (3R,6R)-rel- (CA INDEX NAME)

Relative stereochemistry.

RN 869114-04-5 CAPLUS

CN D-arabino-Hexitol, 1,5-anhydro-2,4,6-trideoxy-2-[[(4-methoxyphenyl)methyl]amino]-6,6-diphenyl-, ethanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 862647-22-1 CMF C26 H29 N O3

Absolute stereochemistry. Rotation (-).

CM 2

CRN 144-62-7 CMF C2 H2 O4

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN

AN 2004:916847 CAPLUS

DN 142:32455

TI Structural requirements for 2,4- and 3,6-disubstituted pyran biomimetics of cis-(6-benzhydryl-piperidin-3-yl)-benzylamine compounds to interact with monoamine transporters

AU Zhang, Shijun; Zhen, Juan; Reith, Maarten E. A.; Dutta, Aloke K.

CS Department of Pharmaceutical Sciences, Wayne State University, Detroit, MI, 48202, USA

SO Bioorganic & Medicinal Chemistry (2004), 12(23), 6301-6315 CODEN: BMECEP; ISSN: 0968-0896

PB Elsevier Ltd.

DT Journal

LA English

OS CASREACT 142:32455

AB In our effort to delineate novel pharmacophoric configuration of bioisosteric pyran versions of cis-(6-benzhydryl-piperidin-3-yl)benzylamine derivs. in interacting with the monoamine transporter, further structure-activity relationship study was carried out. Both cis and trans 2,4- and 3,6-disubstituted derivs. were synthesized to determine the positional importance of N-substitution on affinity for monoamine transporters, that is the dopamine transporter (DAT), the serotonin transporter (SERT), and the norepinephrine transporter (NET) in rat brain. For that purpose, the potency of compds. was determined in competing for the binding of [3H]WIN 35,428, [3H]citalopram, and [3H]nisoxetine, resp. Selected compds. were also evaluated for their activity in inhibiting the uptake of [3H]DA by DAT. Our binding results demonstrated potency in 3,6-disubstituted derivs. while 2,4-disubstituted derivs. failed to exhibit any appreciable binding affinity. Further structural exploration of the exocyclic N-atom in 3,6-disubstituted derivs. produced compds. potent at both DAT and NET.

IT 805251-49-4P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(structural requirements for 2,4- and 3,6-disubstituted pyran biomimetics of cis-(6-benzhydryl-piperidin-3-yl)-benzylamine compds. to interact with monoamine transporters)

RN 805251-49-4 CAPLUS

CN 2H-Pyran-3-amine, 6-(diphenylmethyl)tetrahydro-N-(phenylmethyl)-, (3R,6R)-rel- (CA INDEX NAME)

Relative stereochemistry.

OSC.G 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT